

The generalized Kondo lattice model and its spin-polaron implementation for cuprates by projection method.

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It is shown that the spin-fermion model found to be an effective low-energy implementation of the three-band Emery model after Wannier transformation of p_x - and p_y -orbitals in the oxygen ions subsystem is reduced to the generalized Kondo lattice model. Its essential feature is the presence of spin-correlated hoppings of the current carriers between distant cells. Numerical calculations of the spin-polaron spectrum demonstrate the important role of the distant hoppings.

1. Introduction

The normal phase quasiparticle structure of cuprate high-temperature superconductors and the nature of the low-energy interactions are crucial to establish the Cooper instability mechanism, anomalous temperature dependence of the kinetic coefficients and a number of other unusual properties [1, 2]. The theory of doped 2D antiferromagnet being far from a complete is mainly developed within 2D Hubbard model, generalized t-J-models, three-band Emery (TBE) model [3, 4, 5, 6] and spin-fermion (SF) model. We will not dwell on the first two models, but note that they differ significantly from the SF and TBE models by the fact that their both charge and spin subsystems are formed by the same carriers. Therefore, we will proceed from the more realistic, in our view, SF and TBE models, where the spin system and the system of charge carriers are determined by d - and p - ions respectively.

It is known that in the strong electron correlations regime the Hamiltonian of the TBE model can be reduced to the spin-fermion model [7, 8, 9, 10]. Note that the spin-fermion model even in the simplest consideration allows one to obtain the basic motive of the cuprate's hole spectrum [7, 8], i.e. it appears that the bottom of the carriers spectrum $E(k)$ is near the boundary of the magnetic Brillouin zone $E(k) \sim (\cos(k_x) + \cos(k_y))^2$.

In this paper the Hamiltonians of the TBE and SF models are reduced to the generalized Kondo lattice model, which takes into account the spin-correlated distant hoppings. Based on the comparison of the spectral dependencies of the spin-polaron quasiparticles for the generalized Kondo model and its reduced version (when only the nearest hoppings are left) we argue the importance of the long-range spin-correlated hoppings.

2. The generalized Kondo lattice model

The Hamiltonian of the Kondo lattice model is derived from TBE model for the CuO_2 -plane [3, 4, 5, 6] which in conventional notation is as follows:

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{pd} + \hat{\mathcal{H}}_I, \quad (1)$$

where

$$\begin{aligned} \hat{\mathcal{H}}_{pd} = & \sum_f (\varepsilon_d \hat{n}_f^d + U_d \hat{n}_{f\uparrow}^d \hat{n}_{f\downarrow}^d) + \sum_l (\varepsilon_p \hat{n}_l^p + U_p \hat{n}_{l\uparrow}^p \hat{n}_{l\downarrow}^p) + \\ & + V_{pd} \sum_{f\delta} \hat{n}_f^d \hat{n}_{f+\delta}^p + t^{pd} \sum_{f\delta\sigma} (\vartheta(\delta) d_{f\sigma}^+ p_{f+\delta,\sigma} + H.c.) + \hat{T}, \end{aligned} \quad (2)$$

$$\hat{T} = \sum_{l\Delta\sigma} t \cdot \varrho(\Delta) p_{l,\sigma}^+ p_{l+\Delta,\sigma}, \quad \hat{\mathcal{H}}_I = \frac{I_1}{2} \sum_{fg} S_f S_{f+g} + \frac{I_2}{2} \sum_{fd} S_f S_{f+d}. \quad (3)$$

Here, ε_p and ε_d are energies of a hole on the oxygen ion O and copper ion Cu respectively, U_p and U_d —Coulomb energy of two holes on O and Cu ions, V_{pd} —repulsion energy of two holes at the nearest oxygen and copper sites, t_{pd} —hybridization parameter between adjacent oxygen p — and copper d — orbitals. Vectors l correspond to the positions of O-sites. Vector δ in (2) takes four values: $\pm\delta_x, \pm\delta_y$ ($\delta_x = (a/2, 0), \delta_y = (0, a/2)$) and connects nearest O-sites in positions $f + \delta$ with Cu-site f . Function $\vartheta(\delta)$ takes into account the relationship between the phases of copper and oxygen orbitals in the hybridization processes. For commonly used orbitals the function $\vartheta(\delta)$ takes following values: $\vartheta(\delta) = \mp 1$ at $\delta = (\pm a/2, 0), (0, \pm a/2)$.

The term \hat{T} corresponds to the direct hole hoppings between the nearest oxygen ions with tunneling integral $t\varrho(\Delta)$. Its sign is defined by the function $\varrho(\Delta)$, which depends on the orientation of the line connecting oxygen ions between which the hopping occurs.

Vector Δ runs four values $(\pm a/2, \pm a/2)$ and couple O ion in site l with the nearest to it O ion with site index $l + \Delta$. For chosen oxygen orbital's phases $\varrho(\Delta) = 1$ if $\Delta = \pm(a/2, a/2)$ and $\varrho(\Delta) = -1$ if $\Delta = \pm(a/2, -a/2)$.

The second term $\hat{\mathcal{H}}_I$ in (1) correspond to the superexchange interaction between spins on the nearest and next-nearest ($d = \pm g_x \pm g_y$) sites. $\pm g_x = (\pm a, 0), \pm g_y = (0, \pm a)$ — vectors connecting nearest neighbors of the copper lattice. It is convenient to use frustration parameter p and effective exchange I : $I_1 = (1 - p)I, I_2 = pI, 0 \leq p \leq 1, I > 0$. In this approach it is assumed that when considering the properties of the spin subsystem of copper ions, we can use a two-dimensional (2D) AFM frustrated Heisenberg model with $S = 1/2$. AFM interaction between nearest copper spins in CuO_2 plane is large (order of 0.13 eV $\cong 1500K$ and considerably exceeds the interplane exchange. The interplane exchange is mainly responsible for the long-range order, which is observed in the insulating phase of CuO_2 planes (for La_2CuO_4 the characteristic Neel temperature is $T_N \sim 300$ K). However, at relatively low hole doping the long-range AFM order vanishes in the entire temperature range. Such behavior is reasonably well simulated by introducing frustration [11]. Cluster calculations indicate the presence of a sufficiently large frustration parameter $I_2/I_1 \sim 0.1$ even for the undoped LSCO [12]. In the present work a quantitative analysis of the spin subsystem is carried out in the framework of a spherically symmetric self-consistent theory [13, 14, 15]. The subsystem of spins, localized on copper ions, is considered in a spin-liquid state which is spherically symmetric in spin space. This means that the spin correlation functions $C_r = \langle S_f S_{f+r} \rangle$ satisfy the conditions $C_r = 3 \langle S_f^{x(y,z)} S_{f+r}^{x(y,z)} \rangle, \langle S_f^\alpha \rangle = 0, (\alpha = x, y, z)$.

In the considered below case $U_p = V_{pd} = t = 0, U_d \neq 0$ the three-band Hamiltonian is considerably simplified

$$\hat{\mathcal{H}}_{pd} = \sum_f \left(\sum_\sigma \varepsilon_d \hat{n}_{f,\sigma}^d + U_d \hat{n}_{f\uparrow}^d \hat{n}_{f\downarrow}^d \right) + \sum_{l,\sigma} \varepsilon_p \hat{n}_{l,\sigma}^p + t^{pd} \sum_{f,\delta,\sigma} (\vartheta(\delta) d_{f,\sigma}^+ p_{f+\delta,\sigma} + H.c.). \quad (4)$$

This allows for operators $p_{f+\delta_x,\sigma}^+$ and $p_{f+\delta_y,\sigma}^+$, written in k -representation, by performing a unitary transformation to go to the new operators $\psi_{k,\sigma}^+$ and $\phi_{k,\sigma}^+$ such that $\psi_{f,\sigma}^+$ does not hybridise to the Cu-orbitals.

Let us introduce operators [16, 17, 18, 19]:

$$\begin{aligned}\phi_{k\sigma} &= (s_{kx} p_{k,\delta_x,\sigma} + s_{ky} p_{k,\delta_y,\sigma}) / s_k, \quad \psi_{k\sigma} = (s_{ky} p_{k,\delta_x,\sigma} - s_{kx} p_{k,\delta_y,\sigma}) / s_k, \\ p_{k,\delta_x,\sigma} &= \frac{1}{\sqrt{N}} \sum_f e^{-ikf} p_{f+\delta_x,\sigma}, \quad p_{k,\delta_y,\sigma} = \frac{1}{\sqrt{N}} \sum_f e^{-ikf} p_{f+\delta_y,\sigma}, \\ s_{kx} &= \sin \frac{k_x}{2}, \quad s_{ky} = \sin \frac{k_y}{2}, \quad s_k = \sqrt{s_{kx}^2 + s_{ky}^2}.\end{aligned}\tag{5}$$

Hamiltonian (4) in the representation of operators $\psi_{f,\sigma}^+$, $\phi_{f,\sigma}^+$ reads:

$$\begin{aligned}\hat{\mathcal{H}}_{pd} &= \varepsilon_d \sum_{f,\sigma} \hat{n}_{f,\sigma}^d + U_d \sum_f \hat{n}_{f\uparrow}^d \hat{n}_{f\downarrow}^d + \varepsilon_p \sum_{f,\sigma} (\phi_{f,\sigma}^+ \phi_{f,\sigma} + \psi_{f,\sigma}^+ \psi_{f,\sigma}), \\ \hat{V} &= -2it^{pd} \sum_{f,g,\sigma} (s_{f-g} d_{f\sigma}^+ \phi_{g\sigma} - s_{f-g}^* \phi_{g\sigma}^+ d_{f\sigma}),\end{aligned}\tag{6}$$

where $s_{f-g} = \frac{1}{N} \sum_k e^{ik(f-g)} s_k$.

In the second-order perturbation theory in t^{pd} the Hamiltonian $\hat{\mathcal{H}}_{pd}$ is represented as:

$$\begin{aligned}\hat{\mathcal{H}}_{eff}^\phi &= N(\varepsilon_d - 4\tau) + \tilde{\varepsilon}_\phi \sum_{f,\sigma} \phi_{f,\sigma}^+ \phi_{f,\sigma} + \varepsilon_p \sum_{f,\sigma} \psi_{f,\sigma}^+ \psi_{f,\sigma} - t_g \sum_{f,g,\sigma} \phi_{f,\sigma}^+ \phi_{f+g,\sigma} + \\ &+ 4\tau(1 + \eta) \sum_{f,n,m,\sigma} (s_n s_m^*) \phi_{f-m,\sigma}^+ \Sigma_{\sigma_1,\alpha} S_f^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha \phi_{f-n,\sigma_1},\end{aligned}\tag{7}$$

where notations are introduced:

$$\tau = \frac{(t^{pd})^2}{\varepsilon_{pd}}, \quad \varepsilon_{pd} = \varepsilon_p - \varepsilon_d, \quad \eta = \frac{\varepsilon_{pd}}{U_d - \varepsilon_{pd}}, \quad \tilde{\varepsilon}_\phi = \varepsilon_p + 2\tau(1 - \eta), \quad t_g = \frac{\tau}{2}(1 - \eta).\tag{8}$$

At appropriate for cuprates values of the model parameters [20]: $t^{pd} = 1.3$ eV, $\varepsilon_{pd} = 3.6$ eV and $U_d = 10.5$ eV we get: $\tau = 0.47$ eV, $\eta = 0.52$, $t_g = 0.11$ eV.

The overlapping parameters $(s_n s_m^*)$ are determined only by the geometry of the lattice and decrease rapidly with the increase of the number of coordination sphere in the copper ions lattice n, m :

$$\begin{aligned}(s_0 s_0^*) &= 0.920, \quad (s_1 s_0^*) = (s_g s_0^*) = -0.136, \quad (s_2 s_0^*) = (s_d s_0^*) = -0.022, \\ (s_3 s_0^*) &= (s_{2g} s_0^*) = -0.010, \quad (s_1 s_1^*) = (s_g s_g^*) = 0.020, \quad (s_2 s_1^*) = 0.003.\end{aligned}\tag{9}$$

The last term in (7) describes the current carriers scattering on localized spins followed by spin flipping, i.e. the Kondo scattering processes. Besides they involve only ϕ -fermion states.

We show that these processes, considering rapid decay of the parameters (9), define the low-energy part of the excitation spectrum, enable to exclude from consideration the ψ -carriers and lead to the justification of the spin-polaron concept. We omit the constant in equation (7) and express it as a sum of single-site terms and terms describing the ϕ -holes motion:

$$\begin{aligned}\hat{\mathcal{H}}_{eff}^\phi &= \tilde{\varepsilon}_\phi \sum_{f,\sigma} \phi_{f,\sigma}^+ \phi_{f,\sigma} + \hat{J}_{\phi-d} + \varepsilon_p \sum_{f,\sigma} \psi_{f,\sigma}^+ \psi_{f,\sigma} + \hat{t}_g^\phi + \hat{t}^{SC}, \\ \hat{J}_{\phi-d} &= J_{\phi-d} \sum_{f,\sigma} \phi_{f,\sigma}^+ \Sigma_{\sigma_1,\alpha} S_f^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha \phi_{f,\sigma_1} = 2J_{\phi-d} \sum_f \vec{S}_f \vec{S}_f^\phi, \\ J_{\phi-d} &= 4\tau(1 + \eta)(s_0 s_0^*), \quad \hat{t}_g^\phi = -t_g \sum_{f,g,\sigma} \phi_{f,\sigma}^+ \phi_{f+g,\sigma}, \\ \hat{t}^{SC} &= 4\tau(1 + \eta) \sum_{f,n,m,\sigma} (1 - \delta_{m,0} \delta_{n,0}) (s_n s_m^*) \phi_{f-m,\sigma}^+ \Sigma_{\sigma_1,\alpha} S_f^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha \phi_{f-n,\sigma_1}.\end{aligned}\tag{10}$$

In the expression for \hat{t}^{SC} the factor $(1 - \delta_{m,0}\delta_{n,0})$ ensures that under the sum there is no the term in which all three sites are the same, i.e. \hat{t}^{SC} corresponds to the motion of a hole with spin flipping.

The biggest in the effective Hamiltonian (10) is the $\phi - d$ -exchange on-site interaction $\hat{J}_{\phi-d}$ with parameter $2J_{\phi-d} = 8\tau(1 + \eta)(s_0 s_0^*)$. It leads to the formation of two energy levels at each site. The lower level corresponds to $\phi - d$ singlet state, with energy $\tilde{\varepsilon}_\varphi^- = \tilde{\varepsilon}_\phi - \frac{3}{2}J_{\phi-d}$ and with wave function $|\varphi_f\rangle = \varphi_f^+|O\rangle$, where $\varphi_f^+ = \frac{1}{\sqrt{2}}(\phi_{f,+}^+ Z_f^{-0} + Z_f^{+0} \phi_{f,-}^+)$. For the localized spins we use Hubbard operators $Z_f^{\lambda_1 \lambda_2}$, where $|O\rangle$ stands for a vacuum in one-site cluster. The upper three-fold degenerate level $\tilde{\varepsilon}_\chi^+ = \tilde{\varepsilon}_\phi + \frac{1}{2}J_{\phi-d}$ corresponds to the three $\phi - d$ triplet states with wave functions:

$$|\chi_{f,m}\rangle = \chi_{f,m}^+|O\rangle, \quad m = -1, 0, 1, \quad (11)$$

$$\chi_{f,0}^+ = \frac{1}{\sqrt{2}}(\phi_{f,+}^+ Z_f^{-0} - Z_f^{+0} \phi_{f,-}^+), \quad \chi_{f,+1}^+ = \phi_{f,+}^+ Z_f^{-0}, \quad \chi_{f,-1}^+ = \phi_{f,-}^+ Z_f^{-0}.$$

The discussed level splitting is qualitatively similar to that which occurs in considering the Zhang-Rice polaron [21].

To justify the spin polaron concept we first define the separation $\Delta_{\varepsilon_p=\varepsilon_\psi; \tilde{\varepsilon}_\varphi^-} = \varepsilon_p - \tilde{\varepsilon}_\varphi^-$ between ε_ψ and $\tilde{\varepsilon}_\varphi^-$ levels:

$$\Delta_{\varepsilon_p=\varepsilon_\psi; \tilde{\varepsilon}_\varphi^-} = \varepsilon_p - \tilde{\varepsilon}_\varphi^- = \varepsilon_p - \tilde{\varepsilon}_\phi + \frac{3}{2}J_{\phi-d} \approx 2\tau[5 + 7\eta]. \quad (12)$$

The low-frequency part of the hole spectrum will be formed near the lower one-site level $\tilde{\varepsilon}_\varphi^-$ and should be determined primarily by the motion of the polaron state $|\varphi_f\rangle \rightarrow |\varphi_{f+g}\rangle$. If the half-width of the band W of this movement due to terms \hat{t}_g^ϕ and \hat{t}^{SC} (10) will be less than $\Delta_{\varepsilon_p=\varepsilon_\psi; \tilde{\varepsilon}_\varphi^-}$, then we are allowed to omit from consideration the ψ carriers.

The bandwidth $2W$ of this motion should indicate a polaron narrowing and, in any case, must be proportional to the spin-spin correlation function $C_g = \langle \vec{S}_f \vec{S}_{f+g} \rangle \simeq 0.2 \div 0.3$ (a typical value for 2D AFM in the spin-liquid state). This is evident from the fact that the motion $|\varphi_f\rangle \rightarrow |\varphi_{f+g}\rangle$ is always associated with a combination of operators $\hat{\varphi}_{f+g}^+ \hat{\varphi}_f$, containing the spin operators at the neighboring sites.

The half-width of the band W_g , generated by the term \hat{t}_g^ϕ (10), is estimated as:

$$W_g = 2t_{gg} = 2\frac{\tau}{2}(1 - \eta)_g = \tau(1 - \eta)_g \ll \Delta_{\varepsilon_p=\varepsilon_\psi; \tilde{\varepsilon}_\varphi^-} \approx 2\tau[5 + 7\eta],$$

i.e. $W_g \ll \Delta_{\varepsilon_p=\varepsilon_\psi; \tilde{\varepsilon}_\varphi^-}$.

The half-width of the band W_{SC} , induced by \hat{t}^{SC} in (10), is defined by the term:

$$\begin{aligned} \hat{t}_g^{SC} &= t_g^{SC} \left[\sum_{f,g,\sigma} \phi_{f+g,\sigma}^+ \Sigma_{\sigma_1,\alpha} S_f^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha \phi_{f,\sigma_1} + \sum_{f,g,\sigma} \phi_{f,\sigma}^+ \Sigma_{\sigma_1,\alpha} S_f^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha \phi_{f+g,\sigma_1} \right] = \\ &= t_g^{SC} \left[\sum_{f,g,\sigma} \phi_{f+g,\sigma}^+ \Sigma_{\sigma_1,\alpha} S_f^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha \phi_{f,\sigma_1} + H.c. \right], \quad t_g^{SC} = 4\tau(1 + \eta)(s_0 s_g^*), \end{aligned} \quad (13)$$

which in \hat{t}^{SC} contains the maximum overlapping $(s_0 s_g^*) = -0.136$ (see. formula (9)). Parameter t_g^{SC} 13 times smaller than the constant of $\phi - d$ -exchange coupling $2J_{\phi-d}$. Taking into account the factor C_g this leads to inequality

$$W_{SC} \ll \Delta_{\varepsilon_p=\varepsilon_\psi; \tilde{\varepsilon}_\varphi^-}. \quad (14)$$

Thus we have: $W_g \ll \Delta_{\varepsilon_p=\varepsilon_\psi;\tilde{\varepsilon}_\varphi^-}$, $W_{SC} \ll \Delta_{\varepsilon_p=\varepsilon_\psi;\tilde{\varepsilon}_\varphi^-}$, which are the consequence of inequalities $J_{\phi-d} \gg t^{SC} \gg t_g$. These conditions mean that in the model (10), we can omit the term $\varepsilon_p \sum_{f,\sigma} \psi_{f,\sigma}^+ \psi_{f,\sigma}$ and introduce the spin-polaron concept.

In the approximation of a small number of ϕ -holes after performing transformation to the Hubbard projection operators $\phi_{f,\sigma}^+ \Rightarrow X_f^{\sigma 0}$, the Hamiltonian (10) takes the form of the Kondo lattice Hamiltonian:

$$\begin{aligned} \hat{\mathcal{H}}_{eff}^K = & \tilde{\varepsilon}_\phi \sum_{f\sigma} X_f^{\sigma 0} X_f^{0\sigma} + 2J_{\phi-d} \sum_f \vec{S}_f \vec{S}_f^\phi - t_g \sum_{f,g,\sigma} X_f^{\sigma 0} X_{f+g}^{0\sigma} + \\ & + 4\tau(1+\eta) \sum_{f,m,n,\sigma} (1 - \delta_{m,0}\delta_{n,0}) (s_n s_m^*) X_{f-m}^{\sigma 0} (\Sigma_{\sigma_1,\alpha} S_f^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha X_{f-n}^{0\sigma_1}). \end{aligned} \quad (15)$$

If in the expression (15) the distant spin-correlated hoppings in the first approximation are ignored (i.e. only the terms with $(s_0 s_g^*)$ are left), we arrive at the Hamiltonian of the reduced Kondo lattice model:

$$\begin{aligned} \hat{\mathcal{H}}_{eff}^{Kr} = & \tilde{\varepsilon}_\phi \sum_{f,\sigma} X_f^{\sigma 0} X_f^{0\sigma} + 2J_{\phi-d} \sum_f \vec{S}_f \vec{S}_f^\phi - t_g \sum_{f,g,\sigma} X_f^{\sigma 0} X_{f+g}^{0\sigma} + \\ & + t_g^{SC} [\sum_{f,g,\sigma} \phi_{f+g,\sigma}^+ \Sigma_{\sigma_1,\alpha} S_f^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha \phi_{f,\sigma_1} + H.c.]. \end{aligned} \quad (16)$$

On the basis of this model in the works [22, 23] the spectral properties of the Fermi quasi-particles in cuprate superconductors were studied.

The description of excitations corresponding to the Hamiltonian (15) is convenient to carry out in the framework of Zwanzig-Mori projection method [24, 25].

3. Basis operators and projection method

Let's introduce three sets of basis operators of charge excitations $A_{j,f,\sigma}$ ($j = 1, 2, 3$), and their Fourier transforms $A_{k,f,\sigma}$:

$$\begin{aligned} A_{1,f,\sigma} &= X_f^{0\sigma}, \quad A_{2,f,\sigma} = \Sigma_{\sigma_1,\alpha} S_f^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha X_f^{0\sigma_1}, \quad A_{3,f,\sigma} = \Sigma_{\sigma_1,\alpha} S_f^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha X_{f+g}^{0\sigma_1}, \\ A_{j,k,\sigma} &= N^{-1/2} \sum_f e^{-ikf} A_{j,f,\sigma}. \end{aligned} \quad (17)$$

Next we consider, related to these operators, the two-time retarded Green's function $G_{ij}(k, t)$ and its Fourier transforms $G_{ij}(k, \omega) = \langle \langle A_{ki} | A_{kj}^+ \rangle \rangle_\omega$ ($i, j = 1, 2, 3$).

To close the equations of motion for $\langle \langle A_{ki} | A_{kj}^+ \rangle \rangle_\omega$:

$$\omega \langle \langle A_{ki} | A_{kj}^+ \rangle \rangle_\omega = K_{ij} + \langle \langle [A_{ki}, \hat{\mathcal{H}}_{eff}^{Kr}] | A_{kj}^+ \rangle \rangle_\omega, \quad (18)$$

it is required to calculate the energy matrix: $D_{ij} = \langle \langle [A_{ik}, \hat{\mathcal{H}}_{eff}^{Kr}], A_{jk}^+ \rangle \rangle$, and the matrix: $K_{ij} = \langle \langle A_{ik}, A_{jk}^+ \rangle \rangle$. Then the Fermi Green's functions are obtained from the set of equations having matrix form $G = (\omega - DK^{-1})^{-1} K$, and the spectrum of Fermi excitations is determined by the poles of the Green's functions: $G_{ij}(k, \omega) = \sum_{n=1}^3 \frac{z_{(i,j)}^n(k)}{\omega - E_n(k)}$, ($i, j = 1, 2, 3$).

Thus, the problem of finding spectrum $E_n(k)$ and residues $z_{(i,j)}^n(k)$ is reduced to the calculation of the matrix elements K_{ij} and D_{ij} . To calculate these elements we denote the terms in the Hamiltonian (16), contributing to the matrix D , by: \hat{J} , \hat{t} , $\hat{\tau}^{(SC)}$ and $\hat{\varepsilon}$.

Using relation

$$\langle \tilde{S}_{f_1} \tilde{S}_{f_2} \tilde{S}_{f_3} \rangle = -\delta_{f_1,f_2} C_{f_1-f_3} - \delta_{f_2,f_3} C_{f_1-f_2} + \delta_{f_1,f_3} C_{f_1-f_2}, \quad (19)$$

that is fulfilled when averaged over a singlet state of the undoped CuO₂-plane, as well as the identity

$$\sum_f s_{f-n} s_{f-m}^* = \delta_{m,n} - \frac{1}{4} \sum_g \delta(m-n-g), \quad (20)$$

where g runs over nearest neighbors, we find the expressions for the matrix elements of operators of the matrix D ($D_{ij} = J_{ij} + t_{ij} + \tau_{ij}^{(SC)} + \varepsilon_{ij} = D_{ji}$):

$$\begin{aligned} J_{11} &= 0; \quad J_{12} = J \frac{3}{8}; \quad J_{31} = 2JC_1\gamma_1; \quad J_{22} = -J \frac{3}{8}; \quad J_{32} = -2JC_1\gamma_1; \quad J_{33} = 2JC_1; \quad (21) \\ \tau_{11}^{(SC)} &= 0; \quad \tau_{12}^{(SC)} = t^{SC}(3 + 4C_1)\gamma_1; \quad \tau_{13}^{(SC)} = 4 t^{SC} \left(\frac{3}{4} + 4C_1\gamma_1^2 + 2C_2\gamma_2 + C_3\gamma_3 \right); \\ \tau_{22}^{(SC)} &= -t^{SC} 8 C_1\gamma_1; \quad \tau_{23}^{(SC)} = -4 t^{SC} \left(\frac{3}{4} - C_1 + 2C_2\gamma_2 + C_3\gamma_3 \right); \quad \tau_{33}^{(SC)} = -t^{SC} 32 C_1\gamma_1; \\ t_{11} &= -4 t \gamma_1; \quad t_{22} = -4 t C_1\gamma_1; \quad t_{32} = -t (3 + 8C_2\gamma_2 + 4C_3\gamma_3); \\ t_{33} &= -4 t (9C_1\gamma_1 + 6C_4\gamma_4 + C_6\gamma_6); \quad t_{12} = t_{13} = 0; \\ \varepsilon_{11} &= \bar{\varepsilon}_p; \quad \varepsilon_{22} = \bar{\varepsilon}_p \frac{3}{4}; \quad \varepsilon_{32} = \bar{\varepsilon}_p 4 C_1 \gamma_1; \quad \varepsilon_{12} = \varepsilon_{13} = 0, \quad \varepsilon_{33} = 4\bar{\varepsilon}_p \left(\frac{3}{4} + 2C_2\gamma_2 + C_3\gamma_3 \right), \end{aligned}$$

where $\gamma_1 = (\cos(k_x) + \cos(k_y))/2$, $\gamma_2 = \cos(k_x) \cos(k_y)$, $\gamma_3 = (\cos(2k_x) + \cos(2k_y))/2$,
 $\gamma_4 = (\cos(2k_x) \cos(k_y) + \cos(2k_y) \cos(k_x))/2$, $\gamma_6 = (\cos(3k_x) + \cos(3k_y))/2$.

For matrix elements of the matrix K we have:

$$K_{11} = 1, \quad K_{12} = K_{13} = 0, \quad K_{22} = \frac{3}{4}, \quad K_{32} = 4C_1\gamma_1, \quad K_{33} = 3 + 8 C_2\gamma_2 + 4C_3\gamma_3. \quad (22)$$

A similar procedure may be used for unreduced Hamiltonian (15). Let us represent matrix elements of the corresponding energy matrix in the form: $D_{ij}^K = \mathcal{J}_{ij} + t_{ij} + \varepsilon_{ij}$, where terms t_{ij} and ε_{ij} equal to the ones calculated earlier in (21), and element \mathcal{J}_{ij} takes into account all the interactions in $\hat{\mathcal{H}}_{eff}^K$ due to localized spin operators $S_f^{x(y,z)}$. The calculation of \mathcal{J}_{ij} ($i, j = 1, 2, 3$) yields ($\lambda_f = \sum_g s_{f+g}$):

$$\begin{aligned} \mathcal{J}_{11} &= 0, \quad \mathcal{J}_{21} = 4\tau(1 + \eta)s_k \sum_f e^{ikf} s_f^* C_f, \quad \mathcal{J}_{31} = 4\tau(1 + \eta)s_k \sum_f e^{ikf} \lambda_f^* C_f, \\ \mathcal{J}_{22} &= 4\tau(1 + \eta) \sum_f (-e^{-ikf} s_f s_0^* - e^{ikf} s_0 s_f^* + |s_f|^2) C_f, \\ \mathcal{J}_{32} &= 4\tau(1 + \eta) \sum_f (-e^{-ikf} s_f \lambda_0^* - e^{ikf} s_0 \lambda_f^* + s_f \lambda_f^*) C_f, \\ \mathcal{J}_{33} &= 4\tau(1 + \eta) \sum_f (-e^{-ikf} \lambda_f \lambda_0^* - e^{ikf} \lambda_0 \lambda_f^* + |\lambda_f|^2) C_f. \end{aligned} \quad (23)$$

Note that, as before, all the matrix elements D_{ij}^K in the low-density limit can be expressed only in terms of the spin-spin correlation functions.

Let us return to the question of how to choose the operator basis (17). Generally speaking, the intuitive natural choice of the basis is dictated by the equations of motion for the

$\langle\langle A_{ki}|A_{kj}^+\rangle\rangle_\omega$, when on the first step the "bare" hole operator $X_f^{0\sigma}$ is chosen as a basis operator A_{ki} . As a result of commutation $[X_f^{0\sigma}, \hat{\mathcal{H}}_{eff}^{Kr}]$ there appear new types of operators like $\Sigma_{\sigma_1,\alpha} S_f^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha X_{f+g}^{0\sigma_1}$, $\Sigma_{\sigma_1,\alpha} S_f^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha X_f^{0\sigma_1}$. These operators are included in the basis and for them the equations of motion are written again. This procedure continues until a certain stage. In the last step there are always operators beyond the basis. These operators are projected on to the already selected basis.

To clarify the question of what kind of excitation operators remain out of the basis, consider the case of $\hat{\mathcal{H}} = \hat{J} = J \sum_{\sigma,\sigma_1} X^{\sigma 0} (\vec{S}_{\frac{1}{2}} \vec{\sigma}_{\sigma\sigma_1}) X^{0\sigma_1}$. Here and below the site index is omitted. A complete set of operators describing excitations from the two states $|\uparrow\rangle, |\downarrow\rangle$ without holes to the four possible states with a hole (a singlet and three triplet states) yields eight transitions operators. These operators can be classified according to the irreducible representations of the rotation group. As a result, there appear two doublets $\hat{s}1_\sigma^+, \hat{s}2_\sigma^+$ and a quartet $\hat{q}_{-3/2}^+, \dots, \hat{q}_{3/2}^+$, where $\hat{s}1_\sigma^+$ describes a transition to the singlet with a hole, and $\hat{s}2_\sigma^+$ – to the triplet state. The quartet is always related to the triplet state transitions. Operators of these excitations are of the form ($\gamma = \pm 1 = 2\sigma$):

$$\begin{aligned} \hat{s}1_\sigma^+ &= \frac{1}{\sqrt{2}}(X^{\gamma 0} Z^{\bar{\gamma}\bar{\gamma}} - X^{\bar{\gamma} 0} Z^{\gamma\bar{\gamma}}), \quad \hat{s}2_\sigma^+ = \frac{1}{\sqrt{2}}(2X^{\gamma 0} - X^{\gamma 0} Z^{\bar{\gamma}\bar{\gamma}} + X^{\bar{\gamma} 0} Z^{\gamma\bar{\gamma}}), \\ \hat{q}_{\frac{3}{2}}^+ &= X^{+0} Z^{++}, \quad \hat{q}_{\frac{1}{2}}^+ = X^{-0} Z^{+-} + X^{+0} Z^{--} - X^{+0} Z^{++}. \end{aligned} \quad (24)$$

Here we made a transformation to the Hubbard operators for the localized spins. Linear combinations of $\hat{s}1_\sigma^+$ and $\hat{s}2_\sigma^+$ yield $A_{1,\sigma} = X^{0\sigma}$ and $A_{2,\sigma} = \Sigma_{\sigma_1,\alpha} S^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha X^{0\sigma_1}$, besides:

$$[\hat{s}1_\sigma, \hat{J}] = -\frac{3}{4}J \cdot \hat{s}1_\sigma, \quad [\hat{s}2_\sigma, \hat{J}] = \frac{J}{4} \cdot \hat{s}2_\sigma, \quad [\hat{q}_{\frac{3}{2}}, \hat{J}] = \frac{J}{4} \cdot \hat{q}_{\frac{3}{2}}, \quad [\hat{q}_{\frac{1}{2}}, \hat{J}] = \frac{J}{4} \cdot \hat{q}_{\frac{1}{2}}. \quad (25)$$

Thus beyond our basis are four quartet operators $\hat{q}_{-3/2}^+, \dots, \hat{q}_{3/2}^+$.

A similar group analysis can be carried out for the two-site excitation operators and can be used to determine selection rules for the matrix elements.

4. Results and discussion

Figure 1 shows the lower band dispersion curves of the spin-polaron excitations $E_1(k)$, obtained by solving the dispersion equation $\omega - DK^{-1} = 0$ for the three effective Hamiltonians of the Emery model. The solid bold line is calculated for the full effective Hamiltonian (15) using three operators basis (17). The solid thin line represents the excitation spectrum for the reduced effective Hamiltonian (16) with the same basis operators. It is evident that in the $\Gamma - M$ -direction both curves show a dispersion minimum nearby the point $(\pi/2, \pi/2)$ of the Brillouin zone. The essential difference between these curves is the Fermi excitations bandwidth. Analysis of the solid curves in figure 1 shows that neglect of the long-range spin-correlated hole hoppings leads to a significant (almost five times) reduction in the spin-polaron bandwidth.

For comparison, the dashed curve shows the spin-polarons dispersion calculated for the effective spin-polaron Hamiltonian (7), written in terms of p -orbitals (see e.g. [26, 27]). In this case the used three basis operators are:

$$A_{1,f,\sigma} = p_{f+\delta_x,\sigma}, \quad A_{2,f,\sigma} = p_{f+\delta_y,\sigma}, \quad A_{3,f,\sigma} = \Sigma_{\delta,\sigma_1,\alpha} S_f^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha p_{f+\delta,\sigma}. \quad (26)$$

It can be seen that the spin-polaron spectrum obtained earlier in the spin-fermion model is well reproduced by the Kondo lattice model (15) and is not reproduced by the reduced Kondo lattice model (16).

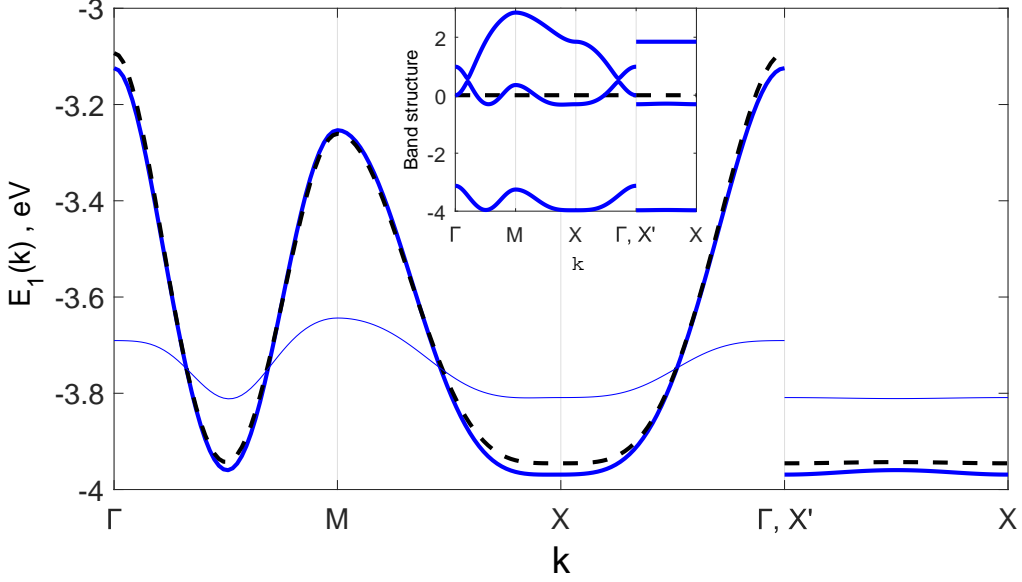


Figure 1: The dispersion curves of the spin-polaron excitations in the lower band for the three effective Hamiltonians of the Emery model. The solid bold curve is for the generalized Kondo lattice Hamiltonian (15), a thin solid line stands for the reduced Kondo lattice model (16) and the dashed curve is the energy spectrum in the spin-fermion model. The calculations were performed for the following values of the pair spin-spin correlation functions: $C_1 = -0.255$, $C_2 = 0.075$, $C_3 = 0.064$ and all C_j with $j > 3$ are zero. For simplicity, we also put $I = 0$. Symmetry points of the Brillouin zone are: $\Gamma = (0, 0)$, $M = (\pi, \pi)$, $X = (\pi, 0)$, $X' = (0, \pi)$. The inset shows the dispersion curves describing three solutions of the cubic dispersion equation $\omega - DK^{-1} = 0$ for the effective Hamiltonian (15) in the basis (17). The lower curve coincides with the bold solid curve of the main figure. Horizontal dashed line in the inset shows the inactive ψ -orbital energy level.

In the inset in the figure 1 by solid lines are shown the three dispersion curves related to the unreduced Kondo-lattice model (15) calculated in the basis of the three operators (17). The horizontal dashed line corresponds to the inactive ψ orbital energy. It can be seen that the lower spin-polaron band is separated from the bare energy of the oxygen p -orbital ε_p (accepted here as zero) down by about 3 eV.

An important feature of the hole spectrum in the cuprate high-temperature superconductors is the absolute minimum nearby the $(\pi/2, \pi/2)$ -point of the Brillouin zone. The dispersion curves in Figure 1 exhibit the minimum only in the direction $\Gamma - M$, but not in the direction $M - M'$. This "incorrect" behavior is due to the fact that when deriving the effective Hamiltonian (15) direct p-p hoppings were rejected. Accounting for these hoppings obviously results in renormalization of the tunneling integral between nearest neighbors t_g , as well as the induction of the new hoppings between distant cells, which intensity is rapidly decreases with increasing the distance.

Consider for example the, largest of the induced, hoppings between next-nearest cells with the tunneling integral t_d . Related to these processes kinetic energy operator

$$\hat{t}^d = -t_d \sum_{f,d,\sigma} \phi_{f\sigma}^+ \phi_{f+d,\sigma} \quad (27)$$

should be added to the Hamiltonians (15) and (16). Thereafter each matrix element D_{ij}

from (21) is renormalized additively on the value of t_{ij}^d ($i, j = 1, 2, 3$). Calculation of the matrix elements t_{ij}^d ($= t_{ji}^d$) gives:

$$\begin{aligned} t_{11}^d &= -4t^d\gamma_2, \quad t_{12}^d = t_{13}^d = 0, \quad t_{22}^d = -4t^dC_2\gamma_2, \quad t_{23}^d = -8t^d(C_1\gamma_1 + C_4\gamma_4), \\ t_{33}^d &= -8t^d(3/4 + 3C_2\gamma_2 + 2C_3\gamma_3 + C_5\gamma_5 + C_7\gamma_7), \end{aligned} \quad (28)$$

where $\gamma_5 = \cos 2k_x \cos 2k_y$, $\gamma_7 = (\cos k_x \cos 3k_y + \cos 3k_x \cos k_y)/2$.

In the figure 2a by solid line is shown the spin polarons spectrum calculated in the three operators basis (17) for the full (unreduced) Kondo lattice Hamiltonian (15) taking into account hoppings between next-nearest neighbors. The dashed line in the same figure shows the spin-polaron spectrum in the reduced Kondo lattice model (16), obtained in the same basis (17) and taking into account the tunneling operator \hat{t}^d . Comparison with the

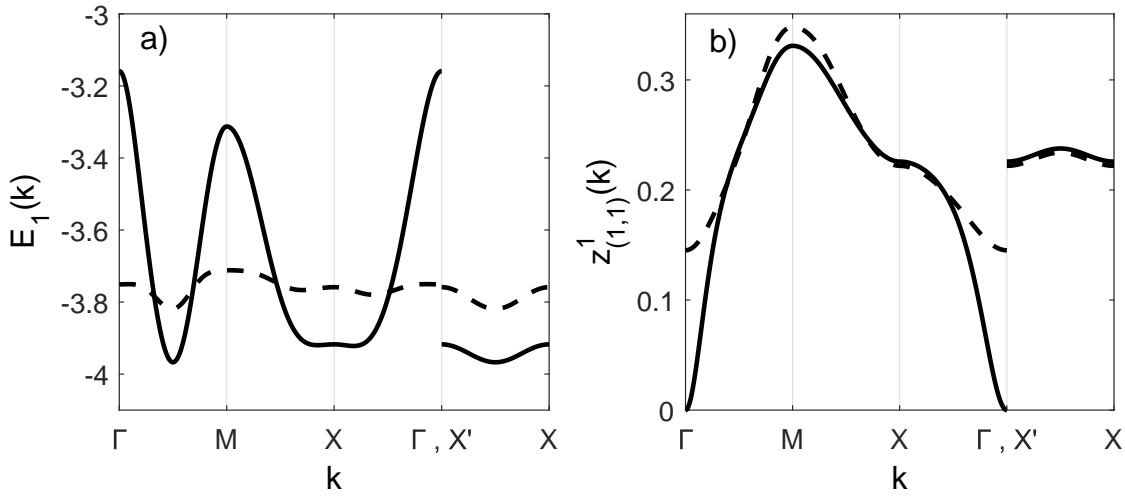


Figure 2: The spectrum (a) and spectral intensity (b) of the lower spin-polaron band calculated taking into account hoppings between next-nearest neighbors. The solid lines correspond to the full generalized Kondo lattice model (15), the dashed line — to the reduced Kondo lattice model (16). In both cases the three operators basis (17) has been used. Tunneling integral $t_d = 0.05$ eV. The rest parameters of the model are the same as in Figure 1.

similar curves in figure 1 shows that the inclusion of p-p-hoppings leads to a minimum in the Fermi excitations spectrum near the $(\pm\pi/2, \pm\pi/2)$ - points of the Brillouin zone, both in the direction $\Gamma - M$ and in the direction $X - X'$. This important fact gives rise at these points to the small hole pockets, which are observed in the experiments on angle-resolved photoelectron spectroscopy in the lightly hole doped high-temperature cuprate superconductors.

Figure 2b shows the wave vector dependence of the residues $z_{(1,1)}^{(1)}(k)$ of the Green's function $G_{11}(k, \omega)$. These residues determine the contribution of the "bare" holes states to the lower spin-polaron state for each value of k . It is seen that in the case of the full Kondo lattice Hamiltonian (15) the "bare" holes contribution to the spin-polaron state vanishes at Γ -point of the Brillouin zone. This behavior is completely consistent with the calculations of the function $z_{(1,1)}^{(1)}(k)$ within the spin-fermion model (i.e., within the effective Hamiltonian (7) written in the representation of the initial oxygen p orbitals) using operator basis (26) [28, 29]. The mentioned feature, however, is not reproduced for the reduced Hamiltonian (16). In this case, as follows from the figure 2b, in the Γ -point of the Brillouin zone the

Green's function residue $z_{(1,1)}^{(1)}(k)$ does not vanish. This fact once again demonstrates the importance of taking into account the distant spin-correlated hoppings.

5. Conclusion

We obtained an effective low-energy Hamiltonian of the three-band Emery model in the form of a generalized Kondo lattice model. An important feature of this Hamiltonian is that it retains the spin-correlated hoppings between distant cells.

Within the generalized Kondo lattice model we analyzed the role of the long-range spin-correlated hoppings which are usually discarded in particular calculations. Comparing the dispersion curves of the spin-polaron spectrum and the spectral density of the "bare" holes calculated for the generalized Kondo lattice model (15) and the reduced Kondo lattice model (16) the essential role of the long-range spin-correlated hoppings is demonstrated. In particular, we show that the retaining of these interactions leads to a significant increase in the spin-polaron bandwidth as well as to an additional reduction of the spin-polaron's minimal energy.

The role of direct oxygen-oxygen hoppings was also analyzed. It was shown that these hoppings are necessary to take into account to reproduce the experimentally observed minimum in the spectrum of spin-polaron excitations in the $(\pm\pi/2, \pm\pi/2)$ -points of the Brillouin zone.

Note that earlier in the Kondo lattice model for two-dimensional doped antiferromagnets the pseudogap behavior of the current carrier's spectral function and anomalous temperature dependence of the kinetic coefficients were considered [30, 31]. However, these studies contained a significant drawback due to ignorance of the hole motion processes with spin-flipping. As a result, in order to achieve a satisfactory agreement between theory and experiment it was necessary to artificially introduce additional hoppings on the first three nearest neighbors, so that the bare band bottom (i.e., without interaction with the spins) was close to the magnetic Brillouin zone boundary. This problem doesn't arise if the low temperature properties of cuprates are studied within the obtained in the work generalized Kondo lattice model (15).

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References

- [1] B. Keimer, S. A. Kivelson, M. R. Norman, S. Uchida, J. Zaanen, *NATURE*, v.**518**, p.179 (2015).
- [2] Nikolay Plakida, *High-Temperature Cuprate Superconductors Experiment, Theory, and Applications*, Springer, 570 pp., 2010.
- [3] V. J. Emery, *Phys.Rev.Lett.* **58**, 2794 (1987).
- [4] C.M. Varma, S. Schmitt-Rink, E. Abrahams, *Solid State Commun.* **62** 681 (1987).
- [5] J.E. Hirsch, *Phys.Rev.Lett.* **59**, 228 (1987).
- [6] V.J. Emery, G. Reiter, *Phys.Rev.B* **38**, 4547 (1988); **38**, 11938 (1988).

- [7] J. Zaanen, A.M. Oles, Phys.Rev.B **37**, 9423 (1988).
- [8] A.F. Barabanov, L.A. Maximov, G.V. Uimin, JETP Lett., **47**, 622 (1988).
- [9] P. Prelovsek, Physics Letters A. **126**, 287 (1988).
- [10] . Matsukawa, H. Fukuyama ,J.Phys.Soc.Jpn. **58**, 2845 (1989).
- [11] M. Inui, S. Doniach and M. Gabay, Phys.Rev.B **38**, 6631 (1988).
- [12] J.F. Annet, R.M. Martin, A.K. McMahan, S. Satpathy, Phys.Rev.B **40**, 2620 (1989).
- [13] J. Kondo, K. Yamaji, Prog. Theor. Phys., **47**, 807 (1972).
- [14] H. Shimahara, S. Takada, J. Phys. Soc. Jpn., **60**, 2394 (1991).
- [15] A.F. Barabanov, V.M. Berezovskii, JETP, **79**, 627 (1994).
- [16] B.S. Shastry, Phys. Rev. Lett. **63**, 1288 (1989).
- [17] J.H. Jefferson, H. Eskes, L.F. Feiner, Phys. Rev. B **45**, 7959 (1992).
- [18] V.A. Gavrichkov, S.G. Ovchinnikov, Physics of the Solid State, **40**, 184 (1998).
- [19] D.F. Digor, V.A. Moskalenko, Theor.Math.Phys., **130**, 320 (2002).
- [20] M. Ogata, H. Fukuyama, Rep.Prog.Phys. **71**, 036501 (2008).
- [21] F.C. Zhang, T.M. Rice, Phys.Rev.B **37**, 3759 (1988).
- [22] A. Ramsak, P. Prelovsek, Phys.Rev.B **40**, 2239 (1989).
- [23] A. Ramsak, P. Prelovsek, Phys.Rev.B **42**, 10415 (1990).
- [24] R. Zwanzig, Phys. Rev. **124**, 983 (1961).
- [25] H.Mori, Prog. Theor. Phys. **33**, 423 (1965).
- [26] A.F. Barabanov, A.A. Kovalev, O.V. Urazaev, A.M. Belemuk, JETP **92**, 677 (2001);
[Rus. ZhETF **119**, 777 (2001)].
- [27] D.M. Dzebisashvili, V.V. Val'kov, A.F. Barabanov, JETP Lett. **98**, 596 (2013).
- [28] R.O. Kuzian, R.Hayn, A.F. Barabanov, L.A. Maksimov, Pys. Rev. B **58**, 6194 (1998).
- [29] V.V. Val'kov, D.M. Dzebisashvili, A.F. Barabanov, Phys. Lett. A. **379**, 421 (2015).
- [30] A.F. Barabanov, A.M. Belemouk, JETP, **111**, 258 (2010).
- [31] I.A. Larionov, A.F. Barabanov, JETP Lett., **100**, 811 (2014).